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CALIFORNIA UNIV LOS ANGELES DEPT OF CHEMISTRY
SYNTHESIS, X-RAY CRYSTAL STRUCTURE AND REACTIONS OF (CLOSO-1,3--ETC(U)
JAN 81 M S DELANEY, R G TELLER, M F HAWTHORNE N00014-76-C-0390
TR-114

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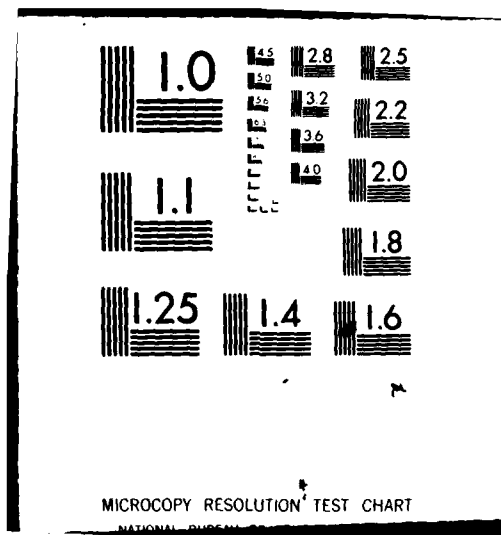
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(9) Interim TECHNICAL REPORT NO. 114

(14) TR-114

(6) SYNTHESIS, X-RAY CRYSTAL STRUCTURE AND REACTIONS OF [closo-1,3,5,2,3-
(1,2,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144,145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,169,170,171,172,173,174,175,176,177,178,179,180,181,182,183,184,185,186,187,188,189,190,191,192,193,194,195,196,197,198,199,200,201,202,203,204,205,206,207,208,209,210,211,212,213,214,215,216,217,218,219,220,221,222,223,224,225,226,227,228,229,230,231,232,233,234,235,236,237,238,239,240,241,242,243,244,245,246,247,248,249,250,251,252,253,254,255,256,257,258,259,260,261,262,263,264,265,266,267,268,269,270,271,272,273,274,275,276,277,278,279,280,281,282,283,284,285,286,287,288,289,290,291,292,293,294,295,296,297,298,299,300,301,302,303,304,305,306,307,308,309,310,311,312,313,314,315,316,317,318,319,320,321,322,323,324,325,326,327,328,329,330,331,332,333,334,335,336,337,338,339,340,341,342,343,344,345,346,347,348,349,350,351,352,353,354,355,356,357,358,359,360,361,362,363,364,365,366,367,368,369,370,371,372,373,374,375,376,377,378,379,380,381,382,383,384,385,386,387,388,389,390,391,392,393,394,395,396,397,398,399,400,401,402,403,404,405,406,407,408,409,410,411,412,413,414,415,416,417,418,419,420,421,422,423,424,425,426,427,428,429,430,431,432,433,434,435,436,437,438,439,440,441,442,443,444,445,446,447,448,449,450,451,452,453,454,455,456,457,458,459,460,461,462,463,464,465,466,467,468,469,470,471,472,473,474,475,476,477,478,479,480,481,482,483,484,485,486,487,488,489,490,491,492,493,494,495,496,497,498,499,500,501,502,503,504,505,506,507,508,509,510,511,512,513,514,515,516,517,518,519,520,521,522,523,524,525,526,527,528,529,530,531,532,533,534,535,536,537,538,539,540,541,542,543,544,545,546,547,548,549,550,551,552,553,554,555,556,557,558,559,560,561,562,563,564,565,566,567,568,569,570,571,572,573,574,575,576,577,578,579,580,581,582,583,584,585,586,587,588,589,590,591,592,593,594,595,596,597,598,599,600,601,602,603,604,605,606,607,608,609,610,611,612,613,614,615,616,617,618,619,620,621,622,623,624,625,626,627,628,629,630,631,632,633,634,635,636,637,638,639,640,641,642,643,644,645,646,647,648,649,650,651,652,653,654,655,656,657,658,659,660,661,662,663,664,665,666,667,668,669,670,671,672,673,674,675,676,677,678,679,680,681,682,683,684,685,686,687,688,689,690,691,692,693,694,695,696,697,698,699,700,701,702,703,704,705,706,707,708,709,710,711,712,713,714,715,716,717,718,719,720,721,722,723,724,725,726,727,728,729,730,731,732,733,734,735,736,737,738,739,740,741,742,743,744,745,746,747,748,749,750,751,752,753,754,755,756,757,758,759,760,761,762,763,764,765,766,767,768,769,770,771,772,773,774,775,776,777,778,779,780,781,782,783,784,785,786,787,788,789,790,791,792,793,794,795,796,797,798,799,800,801,802,803,804,805,806,807,808,809,810,811,812,813,814,815,816,817,818,819,820,821,822,823,824,825,826,827,828,829,830,831,832,833,834,835,836,837,838,839,840,841,842,843,844,845,846,847,848,849,850,851,852,853,854,855,856,857,858,859,860,861,862,863,864,865,866,867,868,869,870,871,872,873,874,875,876,877,878,879,880,881,882,883,884,885,886,887,888,889,890,891,892,893,894,895,896,897,898,899,900,901,902,903,904,905,906,907,908,909,910,911,912,913,914,915,916,917,918,919,920,921,922,923,924,925,926,927,928,929,930,931,932,933,934,935,936,937,938,939,940,941,942,943,944,945,946,947,948,949,950,951,952,953,954,955,956,957,958,959,960,961,962,963,964,965,966,967,968,969,970,971,972,973,974,975,976,977,978,979,980,981,982,983,984,985,986,987,988,989,990,991,992,993,994,995,996,997,998,999,1000,1001,1002,1003,1004,1005,1006,1007,1008,1009,1010,1011,1012,1013,1014,1015,1016,1017,1018,1019,1020,1021,1022,1023,1024,1025,1026,1027,1028,1029,1030,1031,1032,1033,1034,1035,1036,1037,1038,1039,1040,1041,1042,1043,1044,1045,1046,1047,1048,1049,1050,1051,1052,1053,1054,1055,1056,1057,1058,1059,1060,1061,1062,1063,1064,1065,1066,1067,1068,1069,1070,1071,1072,1073,1074,1075,1076,1077,1078,1079,1080,1081,1082,1083,1084,1085,1086,1087,1088,1089,1090,1091,1092,1093,1094,1095,1096,1097,1098,1099,1100,1101,1102,1103,1104,1105,1106,1107,1108,1109,1110,1111,1112,1113,1114,1115,1116,1117,1118,1119,1120,1121,1122,1123,1124,1125,1126,1127,1128,1129,1130,1131,1132,1133,1134,1135,1136,1137,1138,1139,1140,1141,1142,1143,1144,1145,1146,1147,1148,1149,1150,1151,1152,1153,1154,1155,1156,1157,1158,1159,1160,1161,1162,1163,1164,1165,1166,1167,1168,1169,1170,1171,1172,1173,1174,1175,1176,1177,1178,1179,1180,1181,1182,1183,1184,1185,1186,1187,1188,1189,1190,1191,1192,1193,1194,1195,1196,1197,1198,1199,1200,1201,1202,1203,1204,1205,1206,1207,1208,1209,1210,1211,1212,1213,1214,1215,1216,1217,1218,1219,1220,1221,122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SYNTHESIS, X-RAY CRYSTAL STRUCTURE AND REACTIONS OF [closo-1,3-μ-
2,3-μ-(1,2-μ-(η²-3,4-CH₂CH₂C(CH₃)=CHCH₂CH₂CH₂))-3-H-3-PPh₃-3,1,2-
RhC₂B₉H₉], A METALLOCARBABORANE CATALYST.

By

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SUMMARY

→ The synthesis, X-ray crystal structure of the title compound (1) and the initial rates of some alkene hydrogenations catalysed by ^{this compound} (1) are reported.

In addition to our studies of alkene reduction catalysed by [closo-3-H-3,3-(PPh₃)₂-3,1,2-RhC₂B₉H₁₁]¹ (2) we have modified the parent catalyst through synthesis by replacing one triphenylphosphine ligand with a chelating alkene attached to the dicarbollide ligand. We have previously reported the synthesis, structure and reactions of [closo-1,3-μ-(η²-3,4-CH₂=CHCH₂CH₂)-3-H-3-PPh₃-3,1,2-RhC₂B₉H₁₀]² (3) and now report the synthesis, structure and reactions of [closo-1,3-μ-(1,2-μ-(η²-3,4-CH₂CH₂C(CH₃)=CHCH₂CH₂CH₂))-3-H-RhC₂B₉H₉], (1). Complex (1) is a member of the relatively rare hydrido-alkene class of complexes^{2,3} and, to our knowledge, only the second such rhodium complex isolated and structurally characterized².

When an ethanol solution of [RhCl(PPh₃)₃] and a 20% molar excess of Cs⁺[7,8-bis(butenyl)-7,8-C₂B₉H₁₀]⁻⁴ were heated to reflux under nitrogen for 3 hrs. a yellow microcrystalline precipitate was obtained in a 90% yield[†]. This product was recrystallized from CHCl₃-heptane or 1,2-dichloroethane-heptane under an inert atmosphere (m.p. 195-197°C, decomposition). Elemental analysis, n.m.r., and i.r. spectra supported the proposed formula for (1).

Crystal data: (1), monoclinic, space group P2₁/c; a = 9.834 (3), b = 9.615(4), c = 39.291(12) Å, β = 98.72(2)°, U = 2825(1) Å³, D_c = 1.431 g cm⁻³, D_m = 1.361 g cm⁻³ (flotation in aqueous KI)⁵. X-ray intensity data were collected by the θ-2θ scan technique with Mo-Kα radiation (zirconium filter) on a Picker FACS 1 automated

diffractometer equipped with a scintillation counter and pulse height analyser. Of a total of 3403 reflections examined, 1942 had $I > 3\sigma(I)$ and were used in the structure determination. The data were corrected for absorption, Lorentz, and polarization effects. The structure was solved by using heavy-atom methods and refined by full matrix least squares techniques, converging at $R=0.082$ and $R_w=0.096^\dagger$. The molecular structure of (1) is shown in the Figure together with significant bond distances and angles. The two butenyl side chains attached to the dicarbollide ligand have dimerized in a "head to tail" manner and the resulting chelating alkene is bound to the rhodium in such a fashion that C=C bond is nearly parallel to the dicarbollide ligand similar to the bonding in (3)². Such a "head to tail" dimerization of alkenes around a rhodium center has previously been observed by Bennet⁶.

A tetrahydrofuran (THF) solution (1) ($2.72 \times 10^{-3} M$) displayed the following initial rates of the hydrogenation of the following terminal alkenes ($9.84 \times 10^{-2} M$) at $25^\circ C$ [$p(H_2)=585 \text{ mm Hg}$]: $1.1 \times 10^{-3} \text{ mol sec}^{-1}/(\text{mol Rh})$, 3,3-dimethylbut-1-ene; $2.4 \times 10^{-3} \text{ mol sec}^{-1}/(\text{mol Rh})$, trimethylvinylsilane; and $9.1 \times 10^{-4} \text{ mol sec}^{-1}/(\text{mol Rh})$, *n*-butyl acrylate. Under the same conditions (2) exhibited comparable rates⁸ while a THF solution of (3) (1.8×10^{-4}), one of the most reactive homogeneous hydrogenation catalysts reported to date, and the following alkenes ($0.13 M$) displayed the following initial rates: $2.3 \times 10^{-1} \text{ mol sec}^{-1}/(\text{mol Rh})$, trimethylvinylsilane; and $8.9 \text{ mol sec}^{-1}/(\text{mol Rh})$, 3,3-dimethyl but-1-ene at $0^\circ C$ [$p(H_2) = 705 \text{ mm Hg}$]². Complex (1) unlike (3) may be recovered unchanged from THF solutions exposed to hydrogen at 25° or $40^\circ C$ indicating that the chelating alkenyl moiety is not hydrogenated as in (3)². Complex (1) shows no enhancement in the rate of hydrogenation of alkenes over the rates displayed by (2). Complex (1) was also found to catalyse the isomerisation of alkenes but was not active for the hydrogenation of alkynes or for hydroformylation of alkenes.

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† Yield based on Rhodium consumed.

‡ Crystallographic details are available on request.

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FIGURE

Molecular structure of (1). (all hydrogen atoms except the rhodium hydride have been omitted for clarity). Distances from Rh to the attached atoms are H 1.4⁷, P 2.342(5), C₂ 2.239(17), C₁ 2.318(14), B₄ 2.235(20), B₇ 2.205(22), B₈ 2.201(21), C₅ 2.260(15), C₆ 2.317(15) Å and C₅-C₆ 1.459(24), C₅-C₁₀ 1.515(23) Å. Some significant angles are C₅-Rh-C₆ 37.2(6), C₂-Rh-C₅ 82.2(6), C₁-Rh-C₆ 93.3(6), H-Rh-C₅ 79⁷, H-Rh-C₆ 92⁷, H-Rh-P 52⁷, C₅-Rh-P 109.8(4), C₆-Rh-P 93.1(5), C₄-C₅-C₆ 123(2), C₄-C₅-C₁₀ 113(1), C₁₀-C₅-C₆ 117(2), C₅-C₆-C₇ 130(2), H₂C₆-C₅ 116(2)°.

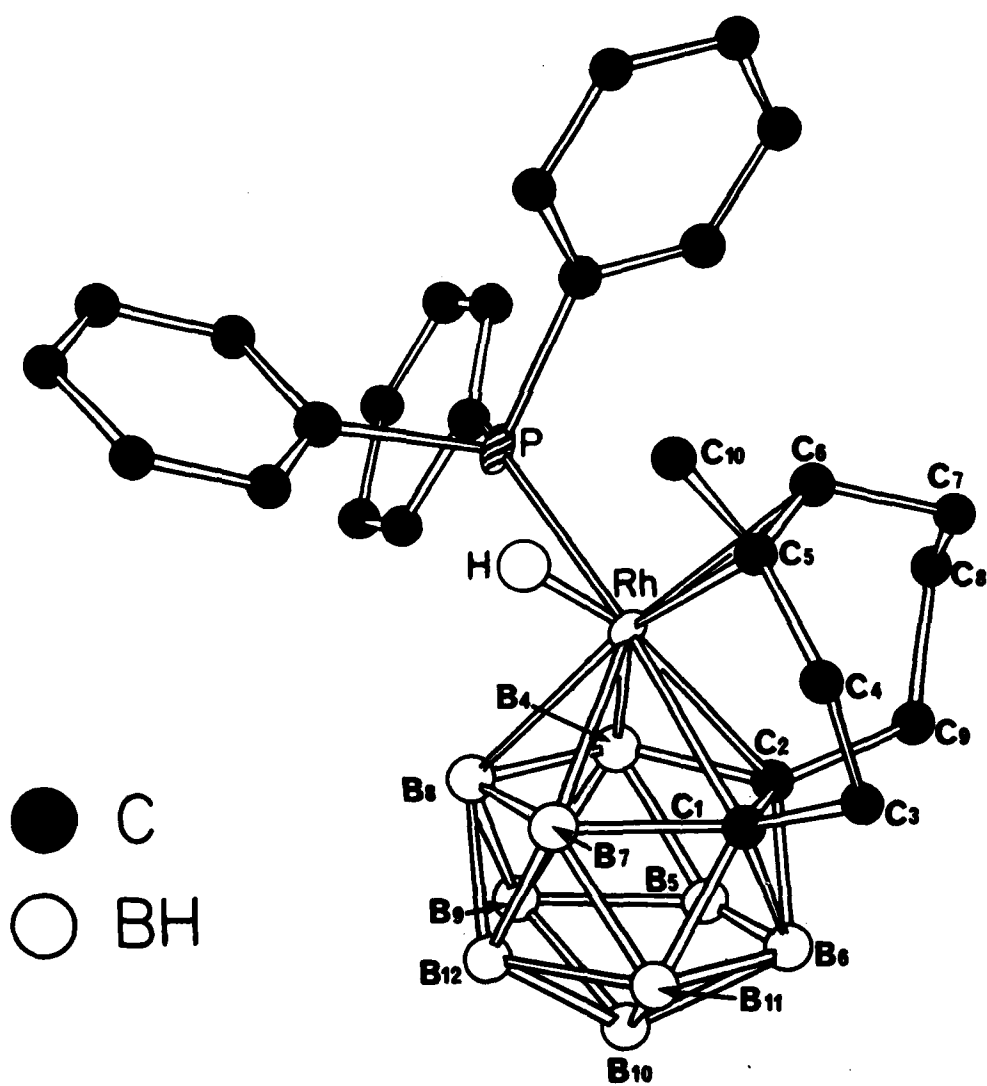


TABLE I**ATOMIC POSITIONS AND TEMPERATURE
FACTORS.**

ATOM	x	y	z	B
HRh	0.0850	0.3100	0.3600	2.00
HC31	0.3095	0.2236	0.2438	2.00
HC32	0.2734	0.3947	0.2290	2.00
HC41	0.0710	0.2327	0.2215	2.00
HC42	0.0513	0.3789	0.2474	2.00
HC6	0.1034	0.0448	0.3349	2.00
HC71	0.2131	-0.0986	0.2822	2.00
HC72	0.2609	0.0435	0.2591	2.00
HC81	0.3729	-0.0053	0.3520	2.00
HC82	0.4407	-0.0921	0.3143	2.00
HC91	0.5742	0.1083	0.3295	2.00
HC92	0.4863	0.1286	0.2798	2.00
H4	0.5000	0.2710	0.4080	2.00
H5	0.6600	0.3100	0.3750	2.00
H6	0.5210	0.3540	0.2750	2.00
H7	0.1530	0.5340	0.3140	2.00
H8	0.2710	0.4690	0.4150	2.00
H9	0.5410	0.5260	0.4250	2.00
H10	0.604	0.625	0.3420	2.00
H11	0.3540	0.6140	0.2720	2.00
H12	0.363	0.695	0.375	2.00

Table II

ATOMIC POSITIONS AND TEMPERATURE
FACTORS^a.

<u>ATOM</u>	<u>x</u>	<u>y</u>	<u>z</u>	<u>B</u>
C2	0.3231(16)	0.3714(19)	0.2978(6)	1.54(35)
C1	0.4278(14)	0.2674(19)	0.3257(5)	1.11(30)
B4	0.4299(21)	0.2986(24)	0.3839(7)	1.89(44)
B5	0.5664(21)	0.3632(25)	0.3571(7)	2.00(44)
B6	0.4951(23)	0.4019(25)	0.3022(8)	2.30(50)
B7	0.2406(20)	0.4891(22)	0.3293(7)	1.51(41)
B8	0.3096(19)	0.4520(23)	0.3867(6)	1.29(40)
B9	0.4879(20)	0.4749(24)	0.3937(7)	1.80(43)
B10	0.5324(22)	0.5356(26)	0.3398(8)	2.51(48)
B11	0.3801(21)	0.5389(23)	0.3031(7)	1.70(44)
B12	0.3770(21)	0.5890(24)	0.3587(7)	1.83(43)

^a Estimated standard deviations, shown in parentheses, refer to the last digit or digits of the preceding number.

Table III

ATOMIC POSITIONS AND TEMPERATURE FACTORS^a ($\times 10^5$)

ATOM	x	y	z	β^{11b}	β^{22}	β^{33}	β^{12}	β^{13}	β^{23}
Rh	0.2412(1)	0.2712(1)	0.34949(4)	376(14)	259(19)	19(1)	10(17)	44(3)	2(6)
P	0.1430(4)	0.1781(5)	0.4138(1)	321(50)	363(70)	17(5)	54(43)	16(13)	3(14)
C3	0.2594(16)	0.3204(18)	0.2518(5)	443(200)	659(291)	23(20)	311(183)	106(54)	6(60)
C4	0.1042(15)	0.2866(21)	0.2492(6)	330(184)	909(306)	53(22)	-48(204)	6(54)	32(74)
C5	0.0647(16)	0.2085(21)	0.2887(5)	499(199)	738(305)	20(19)	-164(210)	-40(52)	70(66)
C6	0.1341(16)	0.0811(19)	0.3061(5)	293(193)	431(271)	32(22)	-305(183)	20(55)	-88(64)
C7	0.2476(19)	-0.0014(18)	0.2891(5)	1085(260)	275(254)	6(20)	143(208)	124(60)	89(58)
C8	0.3881(20)	-0.0036(19)	0.3196(6)	1031(275)	148(262)	57(26)	143(219)	47(71)	13(66)
C9	0.4768(18)	0.1251(20)	0.3130(6)	551(229)	519(291)	47(26)	-12(214)	65(60)	-65(68)
C10	-0.0869(18)	0.2210(24)	0.2926(6)	883(241)	1365(373)	45(22)	-122(258)	75(61)	-159(85)

^a Estimated standard deviations, shown in parentheses, refer to the last digit or digits of the preceding number.

^b The anisotropic temperature factor \underline{I} is defined as $T = \exp[-\{\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl\}]$

Table IV

GROUP PARAMETERS^a

GROUP	X	Y	Z	ϕ	θ	ρ	GROUP B
PHENYL 1	0.0204(9)	0.2896(11)	0.4395(3)	0.079(9)	2.224(6)	2.358(10)	1.60(14)
PHENYL 2	0.2669(10)	0.1365(12)	0.4648(3)	-0.404(6)	3.113(6)	1.067(7)	1.75(15)
PHENYL 3	0.0435(10)	0.0155(9)	0.4027(4)	-2.077(6)	3.122(7)	-0.333(7)	1.83(15)

^a ϕ , θ and ρ are given in radians. For the definition of these terms see C. Scheringer, Acta Cryst., 16, 546 (1963).

Table IV (continued)

GROUP ATOMS - DERIVED POSITIONAL PARAMETERS

Group	Atom	x	y	z
1	1	0.020429	0.289633	0.439509
1	2	-0.007741	0.250022	0.481368
1	3	-0.104953	0.323001	0.501314
1	4	-0.173855	0.435487	0.479372
1	5	-0.145685	0.475098	0.437512
1	6	-0.048473	0.402119	0.417566
1	7	0.041822	0.169122	0.497144
1	8	-0.125086	0.294424	0.531390
1	9	-0.243551	0.487809	0.493672
1	10	-0.195108	0.555893	0.421708
1	11	-0.028200	0.430591	0.387462
2	1	0.266855	0.136490	0.464815
2	2	0.260533	0.009080	0.486253
2	3	0.343266	-0.015134	0.526931
2	4	0.432203	0.088097	0.546112
2	5	0.438524	0.215506	0.524674
2	6	0.355791	0.239720	0.483997
2	7	0.196565	-0.065149	0.472453
2	8	0.338615	-0.106723	0.542295
2	9	0.491519	0.070736	0.575277
2	10	0.502373	0.289770	0.538416
2	11	0.360324	0.331344	0.468574
3	1	0.043532	0.015530	0.402686
3	2	-0.099552	0.016698	0.395896
3	3	-0.172174	-0.102759	0.380727
3	4	-0.101609	-0.223213	0.372371
3	5	0.041475	-0.224381	0.379162
3	6	0.114098	-0.104924	0.394330
3	7	-0.150284	0.103336	0.401907
3	8	-0.274974	-0.101766	0.375863
3	9	-0.153676	-0.308858	0.361496
3	10	0.092312	-0.310848	0.373172
3	11	0.217002	-0.105745	0.399216

Table V**INTER ATOMIC DISTANCES**

<u>Bond Distance</u>	<u>Å</u>	<u>Bond Distance</u>	<u>Å</u>
Rh-H	(1.43) ^a	B5-B9	1.797(30)
Rh-P	2.342(5)	B5-B10	1.753(34)
Rh-C2	2.239(17)	B6-B10	1.720(33)
Rh-C1	2.317(14)	B6-B11	1.737(32)
Rh-C5	2.260(15)	B7-B8	1.805(28)
Rh-C6	2.317(16)	B7-B11	1.748(29)
Rh-B4	2.235(20)	B7-B12	1.775(28)
Rh-B7	2.205(22)	B8-B9	1.747(26)
Rh-B8	2.201(21)	B8-B12	1.748(30)
C2-C3	1.521(23)	B9-B10	1.846(30)
C1-C2	1.584(22)	B9-B12	1.782(29)
C2-B6	1.701(26)	B10-B11	1.728(29)
C2-B7	1.754(27)	B10-B12	1.782(30)
C2-B11	1.703(28)	B11-B12	1.754(29)
C1-B9	1.517(24)	C3-C4	1.549(21)
C1-B4	1.787(26)	C4-C5	1.512(24)
C1-B5	1.795(26)	C5-C6	1.459(24)
C1-B6	1.657(29)	C5-C10	1.515(23)
B4-B5	1.780(30)	C6-C7	1.517(23)
B4-B8	1.897(30)	C7-C8	1.542(25)
B4-B9	1.796(32)	C8-C9	1.542(25)
B5-B6	1.746(31)		
P-Phenyl group(Ave)	1.85(8)		

^aThis atomic position (HRh) was not refined.

Table VI

ANGLES	(°)	ANGLES	(°)	ANGLES	(°)
H-Rh-P	(52) ^a	C1-Rh-C2	40.6(6)	Rh-C1-C9	115.4(11)
H-Rh-C5	(79)	C2-Rh-B4	76.0(7)	Rh-C1-C2	67.0(8)
H-Rh-C6	(92)	C2-Rh-B7	46.5(7)	Rh-C1-B4	64.5(8)
H-Rh-C2	(136)	C2-Rh-B8	79.0(7)	Rh-C1-B5	118.6(10)
H-Rh-C1	(174)	C1-Rh-B4	46.2(6)	Rh-C1-B6	123.9(12)
H-Rh-B4	(130)	C1-Rh-B7	77.3(7)	B4-C1-B5	59.6(11)
H-Rh-B7	(96)	C1-Rh-B8	80.5(6)	B4-C1-B6	110.2(15)
H-Rh-B8	(93)	B4-Rh-B7	82.9(7)	B5-C1-B6	60.6(12)
P-Rh-C2	167.8(4)	B4-Rh-B8	50.6(8)	Rh-B4-C1	69.3(8)
P-Rh-C1	130.4(4)	B7-Rh-B8	48.4(7)	Rh-B4-B5	123.7(13)
P-Rh-B4	92.0(6)	Rh-C2-C1	72.3(8)	Rh-B4-B8	63.8(9)
P-Rh-B7	130.8(6)	Rh-C2-C3	109.2(11)	Rh-B4-B9	116.3(12)
P-Rh-B8	91.8(5)	Rh-C2-B6	126.2(12)	C1-B4-B5	60.4(11)
P-Rh-C5	109.8(4)	Rh-C2-B7	65.7(9)	C1-B4-B8	104.9(14)
P-Rh-C6	93.1(5)	Rh-C2-B11	121.6(12)	C1-B4-B9	106.1(15)
C5-Rh-C6	37.2(6)	C1-C2-C3	115.6(15)	B5-B4-B8	105.4(15)
C5-Rh-C2	82.2(6)	C1-C2-B6	60.4(11)	B5-B4-B9	60.3(12)
C5-Rh-C1	104.6(6)	C1-C2-B7	115.5(14)	B8-B4-B9	56.4(11)
C5-Rh-B4	150.3(7)	C1-C2-B11	111.4(13)	C1-B5-B4	60.0(10)
C5-Rh-B7	96.7(7)	B6-C2-B7	112.2(14)	C1-B5-B6	55.8(11)
C5-Rh-B8	143.4(7)	B6-C2-B11	61.4(12)	C1-B5-B9	105.8(13)
C6-Rh-C2	95.6(6)	B7-C2-B11	60.8(12)	C1-B5-B10	103.2(14)
C6-Rh-C1	93.3(6)	C2-C1-C9	129.6(14)	B4-B5-B6	106.6(14)
C6-Rh-B4	125.2(7)	C2-C1-B4	109.5(14)	B4-B5-B9	60.3(12)
C6-Rh-B7	129.3(7)	C2-C1-B5	110.0(14)	B4-B5-B10	110.0(16)
C6-Rh-B8	173.7(6)	C2-C1-B6	63.3(12)	B6-B5-B9	108.2(15)

Table VI (continued)

ANGLES	(°)	ANGLES	(°)	ANGLES	(°)
B6-B5-B10	58.9(13)	B4-B8-B12	106.2(14)	B6-B11-B7	110.8(16)
B9-B5-B10	62.6(13)	B7-B8-B9	108.7(14)	B6-B11-B10	59.5(13)
C1-B6-C2	56.2(11)	B7-B8-B12	59.9(12)	B6-B11-B12	109.1(16)
C2-B6-B5	107.0(16)	B9-B8-B12	61.3(12)	B7-B11-B10	111.5(16)
C2-B6-B10	107.0(16)	B4-B9-B5	59.4(12)	B7-B11-B12	60.9 (12)
C2-B6-B11	59.4(12)	B4-B9-B8	64.7(12)	B10-B11-B12	61.6(13)
C1-B6-B5	63.6(12)	B4-B9-B10	105.2(15)	B7-B12-B8	61.6(12)
C1-B6-B10	110.9(17)	B4-B9-B12	109.2(14)	B7-B12-B9	108.5(16)
C1-B6-B11	106.3(16)	B5-B9-B8	111.3(15)	B7-B12-B10	107.7(15)
B5-B6-B10	60.8(14)	B5-B9-B10	57.5(12)	B7-B12-B11	59.4(12)
B5-B6-B11	108.4(17)	B5-B9-B12	106.2(15)	B8-B12-B9	59.3(11)
B10-B6-B11	60.0(13)	B8-B9-B10	107.2(14)	B8-B12-B10	110.0(16)
Rh-B7-C2	67.8(9)	B8-B9-B12	59.4(11)	B8-B12-B11	108.7(16)
Rh-B7-B8	65.7(9)	B10-B9-B12	58.8(12)	B9-B12-B10	62.4(12)
Rh-B7-B11	121.1(13)	B5-B10-B6	60.3(13)	B9-B12-B11	107.9(15)
Rh-B7-B12	119.0(13)	B5-B10-B9	59.9(12)	B10-B12-B11	58.5(12)
C2-B7-B8	105.0(14)	B5-B10-B11	108.5(16)	C2-C3-C4	112.5(13)
C2-B7-B11	58.2(11)	B5-B10-B12	108.1(16)	C3-C4-C5	115.5(14)
C2-B7-B12	104.2(13)	B6-B10-B9	107.2(17)	C4-C5-C6	122.6(16)
B8-B7-B11	106.4(13)	B6-B10-B11	60.5(13)	C4-C5-C10	113.1(15)
B8-B7-B12	58.4(11)	B6-B10-B12	108.5(16)	C10-C5-C6	116.8(16)
B11-B7-B12	59.7(11)	B9-B10-B11	106.2(15)	C5-C6-C7	130.0(15)
Rh-B8-B4	65.6(9)	B9-B10-B12	58.8(12)	C6-C7-C8	116.3(14)
Rh-B8-B7	65.9(9)	B11-B10-B12	59.9(12)	C7-C8-C9	112.6(15)
Rh-B8-B9	120.4(13)	C2-B11-B6	59.2(12)	C8-C9-C1	118.8(14)
Rh-B8-B12	120.5(13)	C2-B11-B7	61.1(11)		
B4-B8-B7	105.0(14)	C2-B11-B10	106.6(15)		
B4-B8-B9	58.9(11)	C2-B11-B12	107.4(15)		

^aThis atomic position (HRh) was not refined.

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